Alan McGaughey

Trustee Professor of Mechanical Engineering
Carnegie Mellon University
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Nanoscale Transport Phenomena Laboratory

Professional Experience

Carnegie Mellon University, Pittsburgh, PA, August 2005 -

- Department of Mechanical Engineering: Trustee Professor (2021-) Professor (2014-2021), Associate Professor (2010-2014), Assistant Professor (2005-2010)
- Department of Materials Science and Engineering (courtesy appointment)

University of Florida, Gainesville, FL, August 2004-July 2005

- Post-doctoral fellow in the Department of Materials Science and Engineering. Advisors: Professors Simon R. Phillpot, Susan B. Sinnott, and Judith C. Yang (University of Pittsburgh).

Education

University of Michigan, Ann Arbor, Michigan, September 2000-June 2004

- Ph.D. Thesis: "Phonon transport in molecular dynamics simulations: Formulation and thermal conductivity prediction." Advisor: Professor Massoud Kaviany, Department of Mechanical Engineering.

University of Toronto, Toronto, Ontario, September 1998-August 2000

- Master of Applied Science. Thesis: "The evaporation and stability of a droplet in a finite system." Advisor: Professor Charles A. Ward, Department of Mechanical and Industrial Engineering.

McMaster University, Hamilton, Ontario, September 1994-April 1998

- Bachelor of Engineering, Department of Mechanical Engineering.

Awards

Research and Academics

- Fellow of the American Physical Society, 2021
- Viskanta Fellowship, Purdue University, 2021
- Trustee Professor of Mechanical Engineering, Carnegie Mellon University, 2021
- Invitational Fellowship for Research in Japan, Japan Society for the Promotion of Science, 2021 (declined due to COVID-19 pandemic)
- Fellow of the American Society of Mechanical Engineers, 2016
- American Physical Society Outstanding Referee, 2015
- Harrington Faculty Fellow, University of Texas at Austin, 2012-2013
- Air Force Office of Scientific Research Young Investigator Program, 2009
- University of Michigan Rackham School of Graduate Studies Distinguished Dissertation Award, 2004.
- University of Michigan Rackham School of Graduate Studies Pre-Doctoral Fellowship, 2003-2004
- University of Michigan College of Engineering Distinguished Achievement Award, Department of Mechanical Engineering, 2003 and 2004
- Natural Sciences and Engineering Research Council of Canada Postgraduate Studies B Scholarship (NSERC PGSB), held May 2001-April 2003 at the University of Michigan
- NSERC PGSA, held September 1998-August 2000 at the University of Toronto
- Association of Professional Engineers Gold Medal, McMaster University, May 1998: Highest cumulative average in graduating engineering class ($\sim$400).
- The Iroquois Trophy, McMaster University, May 1998: Highest cumulative average in graduating mechanical engineering class ($\sim$80).
- Canada Scholars Special Corporate Award: Atomic Energy of Canada Limited (AECL) Award, McMaster University, 1997
- Canada Scholarship, held September 1994-April 1998 at McMaster University

Teaching and Service

- Outstanding Mentoring Award, Carnegie Mellon University, 2024
- Philip L. Dowd Fellowship, Carnegie Mellon University, 2019
- Professor of the Year/Best Professor, Mechanical Engineering, Carnegie Mellon University, 2012, 2015, 2017, and 2026 (voted by graduating seniors)
- National Academy of Engineering, Frontiers of Engineering Education Symposium, 2015
- Benjamin Richard Teare Teaching Award, Carnegie Mellon University, 2014
- Struminger Junior Faculty Fellow, Carnegie Mellon University, 2009
- University of Michigan College of Engineering Distinguished Leadership Award, 2004
- Outstanding Graduate Student Instructor Award, University of Michigan, April 2002

Supervision

Post-doctoral fellows: Haibin Chen (2009-2011), Joe Turney (2010)*, Minyoung Lee (2011), Lin Hu (2011-2012), Hasan Babaei# (2015-2018), Manoj Settipalli (2023-2024), Abhishek Pathak+ (2023-2025), Aditya Dey (2025-). Co-advised with: * Cristina Amon, # Chris Wilmer, + Jonathan Malen.

Ph.D. students: Eric Landry (2007-2009), Joe Turney* (2006-2009), John Thomas (2006-2010), Minyoung Lee (2006-2010), Jason Larkin (2009-2013), Wee-Liat Ong+ (2010-2014), Ankit Jain (2011-2015), Shubhaditya Majumdar+ (2011-2016), Ivy Yu (2011-2016), Simon Lu (2011-2016), Francisco Ramirez (2015-2017), Kevin Parrish+ (2013-2017), Henry Aller+ (2016-2021), Hyun-Young Kim (2016-2021), Xiaoman Wang+ (2017-2021), Jie Gong (2017-2022), Holden Parks# (2017-2022), Shuyan Zhang& (2018-2022), Hariharan Ramasubramanian (2021-2026), Ethan Meitz (2022-)%, Nathan Wasserman (2022-)@, Minsung An+ (2024-), Shahid Ahmed+ (2024-), Shubham Deshmukh+ (2024-), Arnab Das+ (2025-), Ben Hroblak (2026-)@. Co-advised with: * Cristina Amon, + Jonathan Malen, # Venkat Viswanathan, & Reeja Jayan, % Gerald Wang, @ Sneha Parra.

Masters students: Eric Landry (2005-2007), Alex Massicotte (2010-2013), Kevin Parrish (2012-2013), Matthew McIntosh (2013-2015), Caroline Gorham (2014-2015), Paarth Thapur (2015-2016), Sushant Kumar (2015-2017), Matthew Bartnof+ (2017-2019), Jinchen Han (2018-2019), Yang Li (2018-2020), Niranjan Bhombe (2022-2024).

Undergraduate students: Sarat Mikkilineni (2006), Madhur Paharia (2006-2007), Takahiro Matsuura (2007), Gary Lee (2007, 2009-2010), Chris Fleck (2008-2010), Ottoleo Kuter-Arnebeck (2008-2009), Nicholas Roche (2008-2009), Ryan Iutzi (2009), Shaun Swanson

(2009-2010), Lucian Cesca (2009), Michael Barako (2009-2010), Gabriella Coloyan (2010-2012), Melanie Jasper (2012), Alex Kowalski (2012), Josh Fuhrman (2014-2015), Justin Abel (2015-2016), Andy Birla (2016-2017), James Zhang (2017), Evan Larrick (2017), Lane Darby (2019), Aaron McKenzie (2019), Rohan Mehta (2020), Michael Pang (2021), Ivy He (2021), Sharon Chu (2021-2022), Daniel Xiao (2020-2023), Zia Reed (2023-2024), Alex Echols (2024), Michael Rapp (2023-2025), Jake Satos (2024-), Sarah Li (2026-).

Visitors: Ryan Iutzi (2009), Dan Sellan (2009), Yusuke Masao (2012), Sam Huberman (2012), Kimmo Saaskilahti (2015), Cheng Shao (2016-2017), I-Ling Chang (2017), Bo Fu (2018-2019), Qi Liang (2019), Jiong Chen (2020), Tomu Hamakawa (2023-2024), Aditya Agarwal (2024).

Contributions to Research

Google Scholar. Citations: 16,253, h-index: 61 (06/05/26)

Book Chapters and Review Articles

6. A. J. H. McGaughey, "Perspective: Twenty-five years of nanoscale thermal transport modeling." *Journal of Materials Science: Materials Theory* **10**, 4 (2026).

5. R. Roy, K. C. Stevens, K. A. Trester, B. S. Sumerlin, A. J. H. McGaughey, J. A. Malen, and A. M. Evans, "Intrinsically thermally conductive polymers." *Materials Horizons* **11**, 3267-3286 (2024).

4. F. DeAngelis, M. G. Muraleedharan, J. Moon, H. R. Seyf, A. J. Minnich, A. J. H. McGaughey, and A. Henry, "Thermal transport in disordered materials." *Nanoscale and Microscale Thermophysical Engineering* **23**, 81-116 (2019).

3. A. J. H. McGaughey, A. Jain, H.-Y. Kim, and B. Fu, "Phonon properties and thermal conductivity from first principles, lattice dynamics, and the Boltzmann transport equation." *Journal of Applied Physics* **125**, 011101 (2019). **Featured Article.**

2. A. J. H. McGaughey and J. M. Larkin, "Predicting phonon properties from equilibrium molecular dynamics simulations." *Annual Review of Heat Transfer Volume 17*, 49-87 (Begell House, 2014).

1. A. J. H. McGaughey and M. Kaviany, "Phonon transport in molecular dynamics simulations: Formulation and thermal conductivity prediction." *Advances in Heat Transfer Volume 39*, 169-255 (Academic Press, 2006).

Journal Publications

121. A. Dey, M. Settipalli, A. M. Evans, and A. J. H. McGaughey, "Layer stacking order tunes thermal and mechanical properties in a prototypical imine-linked 2D covalent organic framework." To appear in *npj Soft Matter*.

120. M. Ohnishi, T. Deng, P. Torres, Z. Xu, T. Tadano, H. Zhang, W. Nong, M. Hanai, Z. Wang, M. Morita, Z. Tian, M. Hu, X. Ruan, R. Yoshida, T. Suzumura, L. Lindsay, A. J. H. McGaughey, T. Luo, K. Hippalgaonkar, and J. Shiomi "Database and deep-learning scalability of anharmonic phonon properties by automated brute-force first-principles calculations." *npj Computational Materials* **12**, 150 (2026).

119. J. Yang, J. Zhu, A. J. H. McGaughey, and W.-L. Ong, "Two distinct phonon wave effects control thermal transport across the coherent–incoherent regime in superlattices." *Advanced Science* **13**, e17251 (2026).

118. A. J. H. McGaughey, L. Lindsay. H. Bao, T. Hamakawa, R. Juneja, S. Li, W. Li, R. Masuki, F. Meng, H. Meng, T. Pandey, C. Shao, J. Shiomi, T. Tadano, A. Togo, A. Wang, and X. Zhang, "Phonon Olympics: Phonon property and lattice thermal conductivity benchmarking from open-source packages." *Journal of Applied Physics* **138**, 135108 (2025). **Featured Article.**

117. K. Kang, A. Pathak, Y. Song, H. Walwil, T. Mirabito, N. S. Mcllwaine, M. Ji, L. S. Larkin, C. B. Saltonstall, A. A. Allerman, J.-P. Maria, J. M. Redwing, J. A. Malen, A. J. H. McGaughey, and S. Choi, "Phonon transport in Al-rich $Al_xGa_{1-x}N$ thin films." *Journal of Applied Physics* **138**, 085101 (2025).

116. T. Hamakawa, A. J. H. McGaughey, and J. Shiomi, "Accurate heat flux formula and thermal conductivity calculation in molecular dynamics simulations with machine learning potentials." *Journal of Applied Physics* **138**, 055105 (2025). **Editor's Pick.**

115. S. Godse, M. Settipalli, J. A. Malen, and A. J. H. McGaughey, "Tacticity-dependent thermal conductivity of single polymer chains." *Applied Physics Letters* **126**, 262201 (2025).

114. N. A. Wassermann, J. P. Miner, J. Shao, T. Sun, A. J. H. McGaughey, and S. P. Narra, "Evolution of powder-entrapped pores in Ti-6Al-4V fabricated with powder bed fusion - laser beam process." *Additive Manufacturing* **109**, 104838 (2025).

113. Y. Liang, K. A. Treaster, A. Majumder, M. Settipalli, K. Panda, S. Godse, R. Roy, R. Mali, Z. Wang, Y. Luan, P. Hu, K. Searles, D. C. McLeod, K. A. Page, D. Bhagwandin, E. Meyhofer, P. Reddy, A. J. H. McGaughey, A. M. Evans, and J. A. Malen, "Anisotropic thermal conductivity in imine-linked 2D polymer films produced by interfacial polymerization." *ACS Nano* **19**, 19009 (2025).

112. J. Yang, X. Zhu, A. J. H. McGaughey, Y. S. Ang, and W.-L. Ong, "Two-mode terms in Wigner transport equation elucidate anomalous thermal transport in amorphous silicon." *Physical Review B* **111**, 094206 (2025).

111. E. J. Meitz, G. J. Wang, and A. J. H. McGaughey, "Phonon mode resolved anharmonic heat capacity of solids." *Physical Review B* **111**, 064305 (2025).

110. H. Ramasubramanian, C. Shao, and A. J. H. McGaughey, "Impact of static disorder and dynamic disorder on the thermal conductivity of sodium superoxide (NaO_2)." *Journal of Applied Physics* **136**, 085104 (2024). **Featured Article.**

109. T. W. Pfeifer, H. Aller, E. R. Hoglund, E. A. Scott, J. A. Tomko, H. Ahmad, A. Doolittle, A. Giri, K. Hattar, A. J. H. McGaughey, and P. E. Hopkins, "Ion irradiation induced crystalline disorder accelerates interfacial phonon conversion and reduces thermal boundary resistance." *Physical Review B* **109**, 165421 (2024).

108. N. A. Wassermann, Y. Li, A. J. Myers, C. A. Kantzos, T. M. Smith, J. L. Beuth, J. A. Malen, L. Shao, A. J. H. McGaughey, and S. P. Narra, "Limits of dispersoid size and number density in oxide dispersion strengthened alloys fabricated with powder bed fusion-laser beam." *Additive Manufacturing* **81**, 104022 (2024).

107. H. T. Aller, A. J. H. McGaughey, and J. A. Malen, "Reduced thermal resistance of amorphous Al_2O_3 thin films on β-Ga_2O_3 and amorphous SiO_2 substrates via rapid thermal annealing." *Applied Physics Letters* **123**, 132202 (2023).

106. L. Su, S. Zhang, A. J. H. McGaughey, B. R. Jayan, and A. Manthiram, "Battery charge curve prediction via feature extraction and supervised machine learning." *Advanced Science* **10**, 2301737 (2023).

105. M.Islamov, P. Boone, H. Babaei, A. J. H. McGaughey, and C. E. Wilmer, "Correlated missing linker defects increase thermal conductivity in metal-organic framework UiO-66." *Chemical Science* **14**, 6592 (2023).

104. S. Zhang, J. Gong, S. Chu, D. Z. Xiao, B. R. Jayan, and A. J. H. McGaughey, "Pair distribution function analysis for oxide defect identification through feature extraction and supervised learning." *APL Machine Learning* **1**, 026115 (2023).

103. M. Islamov, H. Babaei, R. Anderson, K. B. Sezginel, J. R. Long, A. J. H. McGaughey, D. A. Gomez-Gualdron, and C. E. Wilmer. "High-throughput screening of hypothetical metal-organic frameworks for thermal conductivity." *npj Computational Materials* **9**, 11 (2023).

102. S. Zhang, J. Gong, D. Xiao, B. R. Jayan, and A. J. H. McGaughey, "Pair distribution function analysis driven by atomistic simulations: Application to microwave radiation synthesized TiO_2 and ZrO_2." *Computational Materials Science* **218**, 111964 (2023).

101. X. Wang, S. A. Ghaffarizadeh, X. He, A. J. H. McGaughey, and J. A. Malen, "Ultrahigh evaporative heat transfer measured locally in submicron water films." *Scientific Reports* **22**, 22353 (2022).

100. J. J. Wang, J. Gong, A. J. H. McGaughey, and D. Segal, "Simulations of heat transport in single-molecule junctions: Investigations of the thermal diode effect." *Journal of Chemical Physics* **157**, 174105 (2022).

99. J. Gong, S. Chu, R. Mehta, and A. J. H. McGaughey, "XGBoost model for electrocaloric temperature change predictions in ceramics." *npj Computational Materials* **8**, 140 (2022).

98. M. E. DeCoster, H. Babaei, S. S. Jung, Z. Hassan, J. T. Gaskins, A. Giri, E. J. Tiernan, J. A. Tomko, H. Baumgart, P. M. Norris, A. J. H. McGaughey, C. E. Wilmer, E. Redel, G. Giri, and P. E. Hopkins, "Hybridization from guest-host interactions reduces the thermal conductivity of metal organic frameworks." *Journal of the American Chemical Society* **144**, 3603 (2022).

97. A. Giri, A. Evans, M. Rahman, A. J. H. McGaughey, and P. E. Hopkins, "Highly negative Poisson's ratio in thermally conductive covalent organic frameworks." *ACS Nano* **16**, 2843 (2022).

96. X. Wang, M. Jeong, A. J. H. McGaughey, and J. A. Malen, "Reducing the uncertainty caused by the laser spot radius in frequency-domain thermoreflectance measurements of thermal properties." *Review of Scientific Instruments* **93**, 023001 (2022).

95. B. Fu, G. Tang, and A. J. H. McGaughey, "Finite temperature force constants are essential for accurately predicting the thermal conductivity of rutile TiO_2." *Physical Review Materials* **6**, 015401 (2022).

94. H. T. Aller, J. A. Malen, and A. J. H. McGaughey, "Universal model for predicting the thermal boundary conductance of a multilayered-metal–dielectric interface." *Physical Review Applied* **15**, 064043 (2021). **Editor's Suggestion.**

93. A. M. Evans, A. Giri, V. K. Sangwan, S. Xun, M. Bartnof, C. G. Torres-Castanedo, H. B. Balch, M. S. Rahn, N. P. Bradshaw, E. Vitaku, D. W. Burke, H. Li, M. J. Bedzyk, F. Wang, J.-L. Brédas, J. A. Malen, A. J. H. McGaughey, M. C. Hersam, W. R. Dichtel, and P. E. Hopkins, "Thermally conductive ultra-low-k dielectric layers based on two-dimensional covalent organic frameworks." *Nature Materials* **20**, 1142 (2021).

92. C. Shao, W.-L. Ong, J. Shiomi, and A. J. H. McGaughey, "Nano-confinement between graphene walls suppresses the near-wall diffusion of the ionic liquid [BMIM][PF6]." *Journal of Physical Chemistry B* **125**, 4527-4535 (2021).

91. B. Smith, G. Coloyan Fleming, K. Parrish, F. Wen, E. Fleming, K. Jarvis, E. Tutuc, A. J. H. McGaughey, and L. Shi, "Mean free path suppression of low-frequency phonons in SiGe nanowires." *Nano Letters* **20**, 8384-8391 (2020).

90. Q. Liang, M. Bartnof, Y.-L. He, J. A. Malen, and A. J. H. McGaughey, "Fullerene rotational dynamics generate disordered configurations that suppress thermal conductivity in superatomic crystals." *Nanoscale Horizons* **5**, 1524-1529 (2020).

89. H. L. Parks, H.-Y. Kim, V. Viswanathan, and A. J. H. McGaughey, "Uncertainty quantification in first-principles predictions of phonon properties and lattice thermal conductivity." *Physical Review Materials* **4**, 083805 (2020).

88. H. Babaei, M. E. DeCoster, M. Jeong, Z. M. Hassan, T. Islamoglu, H. Baumgart, A. J. H. McGaughey, R. Engelbert, O. K. Farha, P. E. Hopkins, J. A. Malen, and C. E. Wilmer, "Observation of reduced thermal conductivity in a metal-organic framework due to the presence of adsorbates." *Nature Communications* **11**, 4010 (2020).

87. X. Wang, Y. Li, J. A. Malen, and A. J. H. McGaughey, "Assessing the impact of disjoining pressure on thin-film evaporation with atomistic simulation and kinetic theory." *Applied Physics Letters* **116**, 213701 (2020).

86. J. Gong and A. J. H. McGaughey, "Device-level thermodynamic model for an electrocaloric cooler." *International Journal of Energy Research* **44**, 5343 (2020).

85. B. Fu, K. D. Parrish, H.-Y. Kim, G. Tang, and A. J. H. McGaughey, "Phonon confinement and transport in ultrathin films." *Physical Review B* **101**, 045417 (2020).

84. H. T. Aller, X. Yu, A. Wise, R. Howell, A. J. Gellman, A. J. H. McGaughey, and J. A. Malen, "Chemical reactions impede thermal transport across metal/β-Ga_2O_3 interfaces." *Nano Letters* **19**, 8533-8538 (2019).

83. S. K. Jha, N. Nakamura, S. Zhang, L. Su, X. L. Phuah, H. Wang, H. Wang, J. S. Okasinski, A. J. H. McGaughey, B. Reeja-Jayan, "Defect-mediated anisotropic lattice expansion in ceramics as evidence for non-thermal coupling between electromagnetic fields and matter." *Advanced Engineering Materials* **21**, 1900762 (2019).

82. H.-Y. Kim, K. D. Parrish, and A. J. H. McGaughey, "Mapping phonon modes from reduced-dimensional to bulk systems." *Journal of Applied Physics* **126**, 144302 (2019).

81. H. L. Parks, A. J. H. McGaughey, and V. Viswanathan, "Uncertainty quantification in first-principles predictions of harmonic vibrational frequencies of molecules and molecular complexes." *Journal of Physical Chemistry C* **123**, 4072-4084 (2019).

80. E. S. O'Brien, J. C. Russell, M. Bartnof, A. D. Christodoulides, K. Lee, J. A. DeGayner, D. W. Paley, A. J. H. McGaughey, W.-L. Ong, J. A. Malen, X.-Y. Zhu, and X. Roy, "Spontaneous electronic band formation and switchable behaviors in a phase-rich superatomic crystal." *Journal of the American Chemical Society* **140**, 15601-15605 (2018).

79. S. Kumar, C. Shao, S. Lu, and A. J. H. McGaughey, "Contributions of different degrees of freedom to thermal transport in the C_{60} molecular crystal." *Physical Review B* **97**, 140303 (2018).

78. H. Babaei, A. J. H. McGaughey, and C. E. Wilmer, "Transient mass and thermal transport during methane adsorption into the metal-organic framework HKUST-1." *ACS Applied Materials & Interfaces* **10**, 2400-2406 (2018).

77. F. V. Ramirez, S. Shen, and A. J. H. McGaughey, "Near-field radiative heat transfer in graphene plasmonic nanodisk dimers." *Physical Review B* **96**, 165427 (2017).

76. F. V. Ramirez and A. J. H. McGaughey, "Plasmonic thermal transport in graphene nanodisk waveguides." *Physical Review B* **96**, 165428 (2017).

75. K. D. Parrish, J. R. Abel, A. Jain, J. R. Abel, J. A. Malen, and A. J. H. McGaughey, "Phonon-boundary scattering in nanoporous silicon films: Comparison of Monte Carlo techniques." *Journal of Applied Physics* **122**, 125101 (2017).

74. S. Lu and A. J. H. McGaughey, "Thermal conductance of graphene/hexagonal boron nitride heterostructures." *Journal of Applied Physics* **121**, 115103 (2017).

73. S. Majumdar, J. A. Malen, and A. J. H. McGaughey, "Cooperative molecular behavior enhances the thermal conductance of binary self-assembled monolayer junctions." *Nano Letters* **17**, 220-227 (2017).

72. H. Babaei, A. J. H. McGaughey, and C. E. Wilmer, "Effect of pore size and shape on the thermal conductivity of metal-organic frameworks." *Chemical Science* **8**, 583-589 (2017).

71. W.-L. Ong, E. O'Brien, P. Dougherty, D. Paley, C. F. Higgs III, A. J. H. McGaughey, J. A. Malen, and X. Roy, "Orientational order controls crystalline and amorphous thermal transport in superatomic crystals." *Nature Materials* **16**, 83-88 (2017).

70. K. Sääskilahti, J. Oksanen, J. Tulkki, A. J. H. McGaughey, and S. Volz, "Vibrational mean free paths and thermal conductivity of amorphous silicon from non-equilibrium molecular dynamics simulations." *AIP Advances* **6**, 121904 (2016).

69. R. Comin, M. K. Crawford, A. H. Said, N. Herron, W. E. Guise, X. Wang, P. S. Whitfield, A. Jain, X. Gong, A. J. H. McGaughey, and E. H. Sargent, "Lattice dynamics and the nature of structural transitions in organolead halide perovskites." *Physical Review B* **94**, 094301 (2016).

68. J. A. Sierra Suarez, S. Majumdar, A. J. H. McGaughey, J. A. Malen, and C. F. Higgs III, "Morse potential-based model for contacting composite rough surfaces: Formulation and application to self-assembled monolayer junctions." *Journal of Applied Physics* **119**, 145306 (2016).

67. A. Jain and A. J. H. McGaughey, "Thermal transport by phonons and electrons in aluminum, silver, and gold from first principles." *Physical Review B* **93**, 081206(R) (2016)

66. Y.-J. Yu and A. J. H. McGaughey, "Energy barriers for dipole moment flipping in PVDF-related ferroelectric polymers." *Journal of Chemical Physics* **144**, 014901 (2016).

65. Z. Liang, A. Jain, A. J. H. McGaughey, and P. Keblinski "Molecular simulations and lattice dynamics determination of Stillinger-Weber GaN thermal conductivity." *Journal of Applied Physics* **118**, 125104 (2015).

64. A. Jain and A. J. H. McGaughey, "Effect of exchange-correlation on first-principles-driven lattice thermal conductivity predictions of crystalline silicon." *Computational Materials Science* **110**, 115-120 (2015).

63. D. Li and A. J. H. McGaughey, "Phonon dynamics at surfaces and interfaces and its implications in energy transport in nanostructured materials - An opinion paper." *Nanoscale and Microscale Thermophysical Engineering* **19**, 166-182 (2015).

62. S. Majumdar, J. A. Sierra-Suarez, S. N. Schiffres, W.-L. Ong, C. F. Higgs III, A. J. H. McGaughey, and J. A. Malen, "Vibrational mismatch of metal leads controls thermal conductance of self-assembled monolayer junctions." *Nano Letters* **15**, 2985-2991 (2015).

61. S. Lu and A. J. H. McGaughey, "Thermal conductance of superlattice junctions." *AIP Advances* **5**, 053205 (2015).

60. A. Jain and A. J. H. McGaughey, "Strongly anisotropic in-plane thermal transport in single-layer black phosphorene." *Scientific Reports* **5**, 8501 (2015).

59. K. D. Parrish, A. Jain, J. M. Larkin, W. A. Saidi, and A. J. H. McGaughey, "Origins of thermal conductivity changes in strained crystals." *Physical Review B* **90**, 235201 (2014).

58. L. Hu and A. J. H. McGaughey, "Thermal conductance of the junction between single-walled carbon nanotubes." *Applied Physics Letters* **105**, 193104 (2014).

57. K. T. Regner, A. J. H. McGaughey, and J. A. Malen, "Analytical interpretation of non-diffusive phonon transport in thermoreflectance thermal conductivity measurements." *Physical Review B* **90**, 064302 (2014).

56. A. Jain and A. J. H. McGaughey, "Thermal conductivity of compound semiconductors: Interplay of mass density and acoustic-optical phonon frequency gap." *Journal of Applied Physics* **116**, 073503 (2014).

55. D. Guo, J. Gao, Y.-J. Yu, S. Santhanam, G. K. Fedder, A. J. H. McGaughey, and S. C. Yao, "Electrocaloric characterization of a poly(vinylidene fluoride-trifluoroethylene-chlorofluoroethylene) terpolymer by infrared imaging." *Applied Physics Letters* **105**, 031906 (2014).

54. Q. Zhu, C. Fleck, W. A. Saidi, A. J. H. McGaughey, and J. C. Yang, "TFOx: A versatile kinetic Monte Carlo program for simulations of island growth in three dimensions." *Computational Materials Science* **91**, 292-302 (2014).

53. J. M. Larkin and A. J. H. McGaughey, "Thermal conductivity accumulation in amorphous silica and amorphous silicon." *Physical Review B* **89**, 144303 (2014).

52. W.-L. Ong, S. Majumdar, J. A. Malen, and A. J. H. McGaughey, "Coupling and transport of organic and inorganic vibrational states and their thermal transport in nanocrystal arrays." *Journal of Physical Chemistry C* **118**, 7288-7295 (2014).

51. D. Guo, J. Gao, Y.-J. Yu, S. Santhanam, A. Slippey, G. K. Fedder, A. J. H. McGaughey, and S. C. Yao, "Design and modeling of a fluid-based micro-scale electrocaloric refrigeration system." *International Journal of Heat and Mass Transfer* **72**, 559-564 (2014).

50. P. Li, L. Hu, A. J. H. McGaughey, and S. Shen, "Crystalline polyethylene nanofibers with the theoretical limit of Young's modulus." *Advanced Materials* **26**, 1065-1070 (2014).

49. J. M. Larkin, J. E. Turney, A. D. Massicotte, C. H. Amon, and A. J. H. McGaughey, "Comparison and evaluation of spectral energy methods for predicting phonon properties." *Journal of Computational and Theoretical Nanoscience* **11**, 257-264 (2014).

48. S. C. Huberman, J. M. Larkin, A. J. H. McGaughey, and C. H. Amon, "Disruption of superlattice phonons by interfacial mixing." *Physical Review B* **88**, 155311 (2013).

47. L. Hu and A. J. H. McGaughey, "Energy accommodation between noble gases and carbon nanotubes." *Journal of Physical Chemistry C* **117**, 18804-18808 (2013).

46. D. Guo, J. Gao, A. J. H. McGaughey, G. K. Fedder, M. Moran, and S. C. Yao, "Design and evaluation of a MEMS-based Stirling microcooler." *Journal of Heat Transfer* **135**, 111003 (2013).

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44. Y. Wang, B. Qiu, A. J. H. McGaughey, X. Ruan, and X. Xu, "Mode-wise thermal conductivity of bismuth telluride." *Journal of Heat Transfer* **135**, 091102 (2013). **Best Paper, ASME Heat Transfer Division, 2015**.

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33. B. Devine, T.-Z. Shan, Y.-T. Cheng, A. J. H. McGaughey, M. Lee, S. R. Phillpot, and S. B. Sinnott, "Atomistic simulations of copper oxidation and Cu/Cu2O interfaces using charge-optimized many-body potentials." *Physical Review B* **84** 125308 (2011).

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15. J. A. Thomas and A. J. H. McGaughey, "Reassessing fast water transport through carbon nanotubes," *Nano Letters* **8**, 2788-2793 (2008).

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7. A. J. H. McGaughey and M. Kaviany, "Observation and description of phonon interactions in molecular dynamics simulations." *Physical Review B* **71**, 184305 (2005).

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5. A. J. H. McGaughey and M. Kaviany, "Quantitative validation of the Boltzmann transport equation phonon thermal conductivity model under the single-mode relaxation time approximation." *Physical Review B* **69**, 094303 (2004).

4. A. J. H. McGaughey and M. Kaviany, "Thermal conductivity decomposition and analysis using molecular dynamics simulations. Part I. Lennard-Jones argon." *International Journal of Heat and Mass Transfer* **47**, 1783-1798 (2004).

3. A. J. H. McGaughey and M. Kaviany, "Thermal conductivity decomposition and analysis using molecular dynamics simulations. Part II. Complex silica crystals." *International Journal of Heat and Mass Transfer* **47**, 1799-1816 (2004).

2. A. J. H. McGaughey and C. A. Ward, "Stability of a droplet in a finite system: Consideration of the solid-vapor interface." *Journal of Applied Physics* **93**, 3619-3626 (2003).

1. A. J. H. McGaughey and C. A. Ward, "Temperature discontinuity at the surface of an evaporating droplet." *Journal of Applied Physics* **91**, 6406-6415 (2002).

Other Writings

6. R. Guo, B.-Y. Cao, T. Luo, and A. J. H. McGaughey, "Machine learning for thermal transport." *Journal of Applied Physics* **136**, 106401 (2024).

5. A. J. H. McGaughey and D. Mattia, "Materials enabling nanofluidic flow enhancement." *MRS Bulletin*, April 2017, 273-275.

4. A. J. H. McGaughey, "Relaxons heat up thermal transport." Viewpoint in *Physics* **9** 118 (October 17, 2016).

3. B. A. Cola, H. Daiguji, C. Dames, N. Fang, K. Fushinobu, S. Inoue, G. Kikugawa, M. Kohno, S. Kumar, D. Y. Li, J. R. Lukes, J. A. Malen, A. J. H. McGaughey, O. Nakabeppu, K. Pipe, P. Reddy, S. Shen, L. Shi, M. Shibahara, Y. Taguchi, K. Takahashi, T. Yamamoto, and T. Zolotoukhina, "Report on the Seventh U.S.-Japan Joint Seminar on Nanoscale Transport Phenomena-Science and Engineering," *Nanoscale and Microscale Thermophysical Engineering* **17** 25-49 (2013).

2. A. J. H. McGaughey, "Modeling thermoelectric materials and devices." *American Ceramic Society Bulletin* **91**, Volume 3, 34-38 (2012).

1. S. R. Phillpot and A. J. H. McGaughey, "Introduction to thermal transport," *Materials Today*, 18-20, June 2005.

Invited Seminars

46. "Thermal transport in hard and soft materials," Sandia National Laboratories, Albuquerque NM, July 2025.

45. "Atomistic origins of heat capacity and thermal conductivity." Rutgers University, Department of Mechanical and Aerospace Engineering, October 2024.

44. "Atomistic origins of heat capacity and thermal conductivity." University of Florida, Department of Mechanical and Aerospace Engineering, September 2024.

43. "Integrating theory, simulation, machine learning, and experiments to solve heat transfer problems." Stevens Institute of Technology, Department of Mechanical Engineering, November 2022.

42. "Integrating theory, simulation, machine learning, and experiments to solve heat transfer problems." Viskanta Lecture, Purdue University, Department of Mechanical Engineering, November 2021.

41. "Thermal transport in large unit cell crystals." University of Virginia, Department of Mechanical and Aerospace Engineering, October 2020 (virtual).

40. "Phonon transport and confinement in thin films." Dalhousie University, Department of Physics & Atmospheric Science, Halifax, Nova Scotia, Canada, October 2019.

39. "Thermal transport in large unit cell crystals." Massachusetts Institute of Technology, S^3TEC, February 2018.

38. "Atomistic modeling of thermal transport." University of Pittsburgh, Department of Mechanical Engineering and Materials Science, November 2017.

37. "Atomistic modeling of thermal transport." University of California, Los Angeles, Department of Mechanical Engineering, October 2017.

36. "Next generation materials for energy transport and conversion: Growth, characterization, and modeling." Northrop Grumman Next, Redondo Beach, CA, October 2017.

35. "Atomistic modeling of thermal transport." Carnegie Mellon University, Department of Materials Science and Engineering, September 2017.

34. "Thermal transport by phonons and electrons from first principles calculations," University of Tokyo, Department of Mechanical Engineering, June 2017.

33. "Thermal transport in organic-inorganic heterostructures," University of Tokyo, Institute of Industrial Science, June 2017.

32. "Thermal transport in organic-inorganic heterostructures," Pontificia Universidad Catolica de Chile, Department of Mechanical Engineering, Santiago, Chile, January 2017.

31. "Thermal transport in organic-inorganic heterostructures," University of California, San Diego, Department of Mechanical Engineering November 2016.

30. "Thermal transport by phonons and electrons from first principles calculations," Cornell University, Department of Materials Science and Engineering, September 2016.

29. "Thermal transport by phonons and electrons from first principles calculations," University of Colorado, Boulder, Department of Aerospace Engineering Sciences, June 2016.

28. "Thermal transport by phonons and electrons from first principles calculations," Sandia National Laboratories, Albuquerque NM, June 2016.

27. "Phonon properties and thermal conductivity of 3-D and 2-D crystals," Ecole Polytechnique, Paris, France, March 2016.

26. "Thermal transport across organic-inorganic interfaces," Ohio State University, Department of Mechanical and Aerospace Engineering, October 2015.

25. "Nanoscale thermal transport: Formulation for modeling at the atomic scale," "Phonon properties and thermal conductivity of 3-D and 2-D crystals," "Vibrational mode properties and thermal conductivity of disordered solids," and "Thermal transport across organic-inorganic interfaces," Xi'an Jiaotong University, Xi'an, China, September 2015.

24. "Thermal transport across organic-inorganic interfaces," Universite Lyon I, Lyon, France, July 2015.

23. "Thermal transport across organic-inorganic interfaces," Universite de Lorraine, Nancy, France, June 2015.

22. "Phonon properties and thermal conductivity from atomistic calculations," and "Thermal transport across organic-inorganic interfaces," Centrale Superlec, Paris, France, June 2015.

21. "Phonon properties and thermal conductivity from atomistic calculations," University of Michigan, Department of Mechanical Engineering, May 2015.

20. "Thermal transport across organic-inorganic interfaces," University of Toronto, Departments of Mechanical and Electrical & Computer Engineering, April 2015.

19. "Thermal transport across organic-inorganic interfaces," University of Alberta, Department of Chemical and Materials Engineering, July 2014.

18. "Phonon properties and thermal conductivity from atomistic calculations," University of California, Berkeley, Department of Mechanical Engineering, July 2014.

17. "Quantum mechanics-driven prediction of nanostructure thermal conductivity," University of Houston, Department of Mechanical Engineering, February 2013.

16. "Transport phenomena in nanostructures," Carnegie Mellon University, Department of Mechanical Engineering, February 2013.

15. "Quantum mechanics-driven prediction of nanostructure thermal conductivity," University of North Texas, Department of Mechanical and Energy Engineering, January 2013.

14. "Quantum mechanics-driven prediction of nanostructure thermal conductivity," University of Texas Austin, Department of Mechanical Engineering, September 2012.

13. "Quantum mechanics-driven prediction of nanostructure thermal conductivity," Air Force Research Laboratory, Dayton, OH, June 2012.

12. "Thermal transport by phonons in thin films," University of Tokyo, Department of Mechanical Engineering, December 2011.

11. "Thermal transport by phonons in thin films," Rensselaer Polytechnic Institute, Department of Materials Science and Engineering, November 2011.

10. "Thermal transport by phonons in thin films," Vanderbilt University, Department of Mechanical Engineering, October 2011.

9. "Thermal transport by phonons in thin films," Korea Advanced Institute of Science and Technology, Department of Mechanical Engineering, July 2011.

8. "Fluid flow and heat transfer in carbon nanotubes," Columbia University, Department of Mechanical Engineering, October 2009.

7. "Phonon transport in semiconductor superlattices," Georgia Tech, Structural Materials Seminar Series, September 2009.

6. "Nanoscale transport phenomena: Insights from molecular simulation," Carnegie Mellon University, Department of Mechanical Engineering, May 2009.

5. "Water structure and flow inside carbon nanotubes," University of Pittsburgh, January 2009.

4. "Molecular dynamics simulations: Introduction and application to transport problems," Carnegie Mellon University, Process Systems Engineering Seminar, November 2005.

3. "Atomic structure and phonon thermal conductivity: Molecular dynamics investigation in real and phonon spaces," University of Minnesota, Department of Mechanical Engineering, June 2004.

2. "Atomic structure and phonon thermal conductivity: Molecular dynamics investigation in real and phonon spaces," Carnegie Mellon University, Department of Mechanical Engineering, April 2004.

1. "Atomic structure and phonon thermal conductivity: Molecular dynamics investigation in real and phonon spaces," Los Alamos National Laboratory, March 2004.

Invited Conference and Workshop Activities (speaker in bold)

33. **A. J. H. McGaughey**, E. Meitz, and G. J. Wang, "Phonon mode-resolved anharmonic heat capacity of solids." MRS 2025 Spring Meeting, Seattle, WA, April 2025.

32. **A. J. H. McGaughey**, X. Wang, A. Ghaffarizadeh, I. He, and J. A. Malen, "Ultrahigh evaporative heat transfer in submicron water films," 10th US-Japan Joint Seminar on Nanoscale Transport Phenomena, San Diego CA, July 2023.

31. (Keynote) **A. J. H. McGaughey**,"Integrating theory, simulation, machine learning, and experiments to solve heat transfer problems." Oak Ridge Postdoctoral Association Research Symposium, July 2022 (virtual).

30. **A. J. H. McGaughey**, "Ultrahigh evaporative heat transfer measured locally in submicron water films interpreted by a data-driven analysis." International Center for Theoretical Physics meeting on Recent Progress in Thermal Transport Theory and Experiments, June 2022 (virtual).

29. **A. J. H. McGaughey**, H. T. Aller, and J. A. Malen, "Universal model for predicting the thermal boundary conductance of a multilayered-metal/dielectric interface." MRS 2021 Fall Meeting (virtual).

28. **A. J. H. McGaughey**, H. T. Aller, and J. A. Malen, "Universal model for predicting the thermal boundary conductance of a multilayered-metal/dielectric interface." XXIX International Materials Research Congress, August 2021 (virtual).

27. **A. J. H. McGaughey**, Q. Liang, W.-L. Ong, M. Bartnof, Y.-L. He, X. Roy, and J. A. Malen, "Thermal transport and fullerene dynamics in superatomic crystals." MRS 2021 Spring Meeting (virtual).

26. **A. J. H. McGaughey**, H. L. Parks, H.-Y. Kim, and V. Viswanathan, "Quantifying uncertainty in first-principles predictions of molecular vibrational frequencies, phonon properties, and thermal conductivity." APS March Meeting 2021 (virtual).

25. H.-Y. Kim, B. Fu, K. D. Parrish, and **A. J. H. McGaughey**, "Phonon confinement in thin films." Nanoscale Thermal Transport and Heat Localization, Vancouver, BC, August 2018.

24. **A. J. H. McGaughey**, "Next-Generation Atomistic Modeling of Thermal Transport." ITherm 2018, San Diego, CA, May 2018.

23. **A. J. H. McGaughey**, "Phonon transport modeling." IEEE NANO 2017, Pittsburgh, PA, July 2017.

22. S. Kumar, C. Shao, S. Lu, and **A. J. H. McGaughey**, "Degree-of-freedom resolved thermal transport in the C_{60} molecular crystal," 9th US-Japan Joint Seminar on Nanoscale Transport Phenomena, Tokyo, Japan, July 2017.

21. **A. J. H. McGaughey** and **X. Ruan**, "Phonon transport modeling: Formulation, implementation, and applications." Six tutorials given over two sessions. ASME 2016 IMECE, Phoenix, AZ, November 2016.

20. (Keynote) **A. J. H. McGaughey** and A. Jain, "Thermal transport by phonons and electrons from first principles." Fourth International Conference on Computational Methods for Thermal Problems (ThermaComp2016), Atlanta, GA, July 2016.

19. **A. J. H. McGaughey**, "Vibrational mode properties in disordered solids." CECAM worksop on "Advanced thermoelectrics at nanoscale: From materials to devices," Paris, France, July 2015.

18. **A. J. H. McGaughey**, "Vibrational mode properties in disordered solids." 6th International Symposium on Advances in Computational Heat Transfer, Piscataway, NJ, May 2015.

17. **A. J. H. McGaughey**, W. L. Ong, S. Majumdar, and J. A. Malen, "Thermal transport across organic-inorganic interfaces," 8th US-Japan Joint Seminar on Nanoscale Transport Phenomena, Santa Cruz, CA, July 2014.

16. **A. J. H. McGaughey**, "Predicting thermal conductivity from molecular dynamics simulations" and "Predicting phonon properties from molecular dynamics simulations," lectures at 2nd International Conference on Phononics and Thermal Energy Science, Shanghai, China, May 2014.

15. **A. J. H. McGaughey** and A. Jain "Phonon transport in periodic silicon nano porous films," 2nd International Conference on Phononics and Thermal Energy Science, Shanghai, China, May 2014.

14. **A. J. H. McGaughey**, A. Jain, J. M. Larkin, E. S. Landry, S. C. Huberman, C. H. Amon, "Phonon transport in periodic materials with feature sizes of 1 nm to 1 mm." AMERIMECH Symposium on Dynamics of Periodic Materials and Structures, Atlanta, GA, April 2014.

13. **A. J. H. McGaughey** , "Phonon transport in periodic silicon nano porous films," 2nd International Conference on Phononics and Thermal Energy Science, Shanghai, China, May 2014

12. **A. J. H. McGaughey** and A. Shakouti,"Measuring and predicting thermal transport properties," tutorial at the 2013 MRS Spring Meeting, San Francisco, CA, April 2013.

11. **A. J. H. McGaughey**, W. L. Ong, S. Majumdar, and J. A. Malen, "Atomic modeling of thermal transport in hybrid organic-inorganic materials." MRS 2013 Spring Meeting, San Francisco, CA, April 2013.

10. **A. J. H. McGaughey**, W. L. Ong, S. Majumdar, and J. A. Malen, "Atomistic modeling of thermal transport in nanocrystal superlattices and self-assembled monolayer junctions." ASME 2012 IMECE, Houston, TX, November 2012.

9. **A. J. H. McGaughey**, "Combining atomistic calculations and the Boltzmann transport equation to predict nanostructure thermal conductivity." Averaging Methods for Multiscale Phenomena in Engineering Materials Workshop, Pittsburgh PA, April 2012.

8. **A. J. H. McGaughey**, A. Jain, J. E. Turney, D. P. Sellan, and C. H. Amon, "Thermal transport in thin films," 7th US-Japan Joint Seminar on Nanoscale Transport Phenomena, Shima, Japan, December 2011.

7. **A. J. H. McGaughey**, J. E. Turney, J. A. Thomas, H. Chen, R. M. Iutzi, A. D. Massicotte, and C. H. Amon, "Predicting phonon properties using the spectral energy density." Phononics 2011, Santa Fe, NM, May 2011.

6. **A. J. H. McGaughey**, "Predicting phonon properties using lattice dynamics calculations and molecular dynamics simulation." Third International Workshop on Transmission of Information and Energy in Nonlinear and Complex Systems, Singapore, July 2010.

5. **A. J. H. McGaughey** and E. S. Landry, "Thermal transport across semiconductor interfaces and thin films." Spring 2010 MRS Meeting, April 2010, San Francisco, CA.

4. J. A. Thomas, R. M. Iutzi, J. E. Turney, and **A. J. H. McGaughey**, "Coupling between phonons and fluid particles in water/carbon nanotube systems," Micro/Nanoscale Heat and Mass Transfer International Conference, Shanghai, China, December 2009.

3. **J. A. Thomas** and A. J. H. McGaughey, "Water transport through carbon nanotubes: Insights from molecular dynamics simulation." Nanobiophysics, Nanochemistry, Nanomedicine & Nanotoxicology Conference 2009, January 2009, Antigua.

2. **A. J. H. McGaughey** and E. S. Landry, "Exploration of superlattice thermal conductivity tensor design space," Spring 2007 MRS Meeting, San Francisco CA, April 2007.

1. **A. J. H. McGaughey**, "Analysis of phonon transport in superlattices using molecular dynamics simulations." CECAM workshop on "Heat transfer simulation at the atomic scale: New challenges for the future," Lyon, France, September 2006.

Research Funding

As PI

- "Exceptional Figures of Merit for Nanogranular Thermoelectrics." $180,000. Sandia National Laboratories. October 2024-September 2026.
- "Thermal performance of ultra-wide bandgap materials and devices under extreme fields." $1,700,000 (to date). Army Research Office. September 2022-. Co-PIs: J. A. Malen (CMU), S. Choi (Penn State University).
- "Vibrational structure and thermal transport in statically and dynamically disordered crystals." $360,000. National Science Foundation, January 2021 - December 2023.
- "Thermally-stable halide perovskites for photovoltaic energy conversion." $75,000, Wilton E. Scott Institute for Energy Innovation, March 2019-June 2020. Co-PI: J. A. Malen (CMU).
- "Electrocaloric cooling in polymers: Multi-scale modeling and experimental characterization." $360,000. National Science Foundation, August 2016 - July 2019. Co-PI: S. C. Yao (CMU).
- "Thermal transport in large unit cell crystals." $330,000. National Science Foundation, July 2015 - June 2018.
- "Heat transfer enhancement in nanoscale film evaporation." $57,000, Pennsylvania Infrastructure Technology Alliance. January 2014 - May 2015. Other PI: J. A. Malen (CMU), co-PI S. C. Yao (CMU).
- "Phonon transport near and across semiconductor interfaces." $300,000. National Science Foundation, September 2010 - August 2013. Co-PI: Y. Wang (Pittsburgh Supercomputing Center)
- "Quantum mechanics-driven prediction of nanostructure thermal conductivity." $361,640. Air Force Office of Scientific Research (Young Investigator Program), May 2010 - April 2013.
- "IDR: Carbon nanotube aerogels for next-generation thermal management." $965,874. National Science Foundation, September 2009 - August 2012. Co-PIs S. Anna and M. Islam (CMU) and K. Pipe (Michigan).
- "Multiscale modeling of phase change materials." $44,175, Pennsylvania Infrastructure Technology Alliance. January 2009 - May 2010. Co-PI J. Bain (CMU).
- "Atomistic characterization and modeling of deep sub-micron gate oxide breakdown." $64,410. Pennsylvania Infrastructure Technology Alliance. January 2008 - May 2009. Co-PI R. F. Davis (CMU).
- "Kapitza conductance of solid-solid interfaces," $8,790. Berkman Faculty Development Fund, Carnegie Mellon University. January 2006-December 2006.

As co-PI

- "Large format wire based directed energy deposition of high strength aluminum alloys enabled by inoculant additions to promote fine grained, wrought equivalent mechanical behavior to replace forgings and support supply chain agility." $115,000. Sandia National Laboratories. October 2025-September 2026. PI: S. Narra (CMU).
- "Poly-HEATLINE: Polymer HEAT Transfer by Learned INtermolecular Enhancement." $6,250,000. September 2023 - August 2028. PI: J. A. Malen (CMU). Other co-PIs: Austin Evans and Brent Sumerlin (U. Florida), Arthi Jayaraman (U. Delaware), Pramod Reddy (U. Michigan).
- "Electric field- and light-modulated thermal transport in superatomic crystals." $289,999 (CMU portion). NSF. August 2020-July 2023. PI: J. A. Malen (CMU). Other co-PI: Xavier Roy (Columbia).
- "AI driven investigation of the physics of field-matter coupling for materials synthesis." $995,723. DARPA. December 2018-May 2020. PI: A. Singh. Other co-PIs: A. Davis, B. R. Jayan.
- "Physical behavior of layered superatomic crystals." $626,372. Army Research Office. October 2017-September 2020. PI: J. A. Malen (CMU). Other co-PI: Xavier Roy (Columbia).
- "Metal alloys for thermal engineering of advanced electronics." $385,000. Northrup Grumman. August 2016-December 2020. PI: J. A. Malen (CMU). Other co-PI: A. Gellman (CMU).
- "Phosphor conversion matrix with high thermal conductivity for next-generation phosphor-converted LED-based solid state lighting." $1,934,774. Department of Energy. August 2014 - November 2016. PI: M. Bockstaller, nine other co-Pis.
- "GOALI: Thermal transport by phonons in device-grade nitride nanostructures." $430,284. National Science Foundation. September 2011-August 2014. PI: J. A. Malen (CMU). Other co-PI: R. F. Davis (CMU).
- "Stirling microcooler array with elemental in-plane flow." $2,600,000. DARPA, June 2010 - May 2013. PI: G. Fedder (CMU). Other co-PIs: W. Anderson (Active Cooling Technologies), M. Moran (Isotherm), and S. C. Yao (CMU).
- "Multiscale atomistic simulation of metal-oxygen surface interactions: methodological development, theoretical investigation and correlation with experiment." $641,301. Department of Energy, Basic Energy Sciences. October 2007-August 2010. PI: J. Yang (Pittsburgh). Other co-PIs: S. R. Phillpot and S. B. Sinnott (Florida).
- "Multiscale atomistic simulation of metal-oxygen surface interactions: methodological development, theoretical investigation and correlation with experiment." $148,000. Department of Energy, Basic Energy Sciences. January 2006-June 2007. PI: J. Yang (Pittsburgh). Other co-PIs: S. R. Phillpot and S. B. Sinnott (Florida).

Contributions to Education

Teaching at Carnegie Mellon University

Course	Units	Offered	Students/ Response	FCE Course	FCE Instructor
24-739: Molecular Simulation of Materials	12	S06	15/13	4.7	4.8
24-703: Numerical Methods in Mech. Eng.	12	F06	39/30	3.9	4.1
24-739: Molecular Simulation of Materials	12	S07	14/8	4.0	4.3
24-734: Small Scale Heat Transfer	6	S07	7/7	3.9	4.3
24-703: Numerical Methods in Mech. Eng.	12	F07	41/29	4.45	4.72
24-701: Math. Techniques in Mech. Eng.	12	S08	25/20	4.25	4.63
24-322: Heat Transfer	10	F08	101/67	4.26	4.46
24-703: Numerical Methods in Mech. Eng.	12	S09	31/31	4.61	4.84
24-322: Heat Transfer	10	F09	97/80	4.16	4.36
24-623: Molecular Simulation of Materials	12	S10	22/19	4.89	4.89
24-322: Heat Transfer	10	F10	99/82	4.51	4.63
24-623: Molecular Simulation of Materials	12	S11	17/15	4.94	5.00
24-322: Heat Transfer	10	F11	89/67	4.61	4.81
24-623: Molecular Simulation of Materials	12	S12	18/17	4.82	4.89
24-311: Numerical Methods	12	F13	123/99	4.30	4.44
24-101: Fundamentals of Mechanical Eng.	12	S14	129/76	3.72	3.97
24-311: Numerical Methods	12	F14	108/72	4.37	4.51
24-101: Fundamentals of Mechanical Eng.	12	S15	115/57	3.72	4.11
24-623: Molecular Simulation of Materials	12	F15	19/16	4.94	4.94
24-311: Numerical Methods	12	S16	128/85	4.60	4.69
24-623: Molecular Simulation of Materials	12	F16	16/10	4.90	4.90
24-231: Fluid Mechanics	10	S17	172/113	4.29	4.42
24-623: Molecular Simulation of Materials	12	F17	29/23	4.83	5.00
24-231: Fluid Mechanics	10	S18	118/72	4.49	4.61
24-623: Molecular Simulation of Materials	12	F18	32/25	4.92	5.00
24-231: Fluid Mechanics	10	S19	125/71	4.46	4.58
24-703: Numerical Methods in Engineering	12	F19	48/37	4.89	4.97
24-623: Molecular Simulation of Materials	12	S20	20/17	4.83	4.94
24-311: Numerical Methods (R)	12	F20	22/15	4.87	5.00
24-703: Numerical Methods in Engineering (R)	12	F21	43/42	4.64	4.79
24-322: Heat Transfer	10	F22	119/71	4.34	4.48
24-703: Numerical Methods in Engineering	12	S23	36/20	4.35	4.30

R = remote teaching

Course	Units	Offered	Students/ Response	FCE Course	FCE Instructor
24-322: Heat Transfer	10	F24	147/72	4.38	4.25
24-311: Numerical Methods	10	S25	123/60	4.27	4.62
24-322: Heat Transfer	10	F25	131/101	4.49	4.66
24-721: Advanced Thermodynamics	12	S26	15/11	4.55	4.64
24-322: Heat Transfer	10	F26			
24-701: Math. Techniques in Mech. Eng.	12	S27			

Innovation

- Developed the new course 24-623: Molecular Simulation of Materials and taught it ten times. Made a series of videos.
- Created active learning modules for 24-311: Numerical Methods, 24-703: Numerical Methods in Mechanical Engineering, and 23-623: Molecular Simulation of Materials. This work formed the basis for my contribution to the 2015 National Academy of Engineering Frontiers of Engineering Education Symposium.
- As the Struminger Junior Faculty Fellow in 2009, I designed two new laboratory demonstrations for 24-322: Heat Transfer.
- Developed the lecture series "Mechanical Engineering from the Nanometer-Up."

Publications

- A. J. H. McGaughey and J. J. Michalek, "Wiki-based learning in the mechanical engineering classroom," 2008 ASEE Annual Conference and Exposition, June 2008, Pittsburgh, PA.
- E. R. Chan, S. P. Holleran, A. J. H. McGaughey, and C. Rasmussen, "ASEE student chapters: Avenues for promoting future engineering educators," 2004 ASEE Annual Conference and Exposition, June 2004, Salt Lake City, UT.

Previous Experience

- University of Michigan, January-April 2001, September-December 2001. Course: ME330: Thermal & Fluid Sciences II, Graduate Student Instructor (GSI).
- University of Toronto, September 1998-April 2000. Courses: MIE 310: Thermodynamics, MIE 313: Heat Transfer and MIE 100: Dynamics, Teaching Assistant (TA).
- Vice-President, University of Michigan ASEE Graduate Student Chapter, May 2003-May 2004.

Service at Carnegie Mellon University

Mechanical Engineering Department

- Seminar Committee (2006-2008)
- Computer Committee (2006-2010)
- Organizer of qualifier exams: Fall 2010, Spring 2011, Fall 2011, Spring 2012
- Mechanical Engineering Graduate Student Organization advisor (2008-2010)
- Graduate Student Research Conference coordinator (2010, 2011)
- Awards Committee (Chair, 2013-2016)
- Graduate Education Committee (2008-2012, 2015-2020),
  Chair (2016-2020). Major responsibilities and accomplishments as Chair:
  - Manage committee of twelve faculty and two staff
  - Oversee PhD and Masters admissions and programs (400+ students)
  - Led graduate education portion of department external review (2018) and strategic plan (2019-20)
  - Design, approval, and rollout of a new Masters program
  - Institution of a new award for best PhD Dissertation
  - Implementation of a new PhD student annual review process
  - Standardization of policy-related processes (e.g., petitions, degree progress)
  - Adding educational components to Teaching Assistant experience
- Undergraduate Education Committee (2021)
- Faculty Search Committee (Chair) (2022-)

College of Engineering

- Civil & Environmental Engineering faculty search (2006)
- Curriculum Review Committee (2010-2012)
- Strategic Planning Committee (2013)
- Center for Faculty Success, Junior Faculty Lead (2015-2020) Major accomplishments:
  - Design and organization of a new orientation for new faculty members
  - Organize and run sessions for junior faculty applying for early career awards
  - Interviewed faculty and reported back to Dean about mentoring and feedback
  - Run "Bias Busters" sessions to remove unconscious bias and increase diversity
- Dean Evaluation Committee (2018)
- Faculty Chair Elect (2018) and Faculty Chair (2019-2020). Responsibilities:
  - Member of College Awards Committee
  - Attend College Council meetings, where Department Heads present proposed curriculum changes
  - Attend Review of Promotion and Tenure meetings, where Department Heads present cases to the Dean
- Dean Search Advisory Committee (2019)

University

- University Committee on Faculty Appointments Without Indefinite Tenure (2011-2012)
- Physics faculty search (2011-2012)
- Goldwater Award selection committee (2014-2017)
- Berkman Faculty Development Fund selection committee (2016-2018)
- DSF Charitable Foundation selection committee (2017)
- University Committee on Appointments with Indefinite Tenure (2021-2023)

Professional Activities

ASME

- Member (2003-), Fellow (2016)
- *Journal of Heat Transfer* Associate Editor (2015-2018)
  - Special recognition for "Exceptional Service"
- *Journal of Heat Transfer*, Outstanding Reviewer (2011)
- Member, ASME Heat Transfer Division K-8 (Theory and Fundamental Research) Committee (2006-).
- Track organizer, 2013 ASME Summer Heat Transfer Conference.
- Track organizer, 2018 IMECE.
- Session organizer and chair, 2008, 2009, and 2012 ASME Summer Heat Transfer Conferences, 2011 ASME/JSME Thermal Engineering Joint Conference, 2013 IMECE.

APS

- Member (2005-)
- Fellow, Division of Materials Physics (2021). Citation: For significant contributions to the development and advancement of theoretical and computational methods for the determination and fundamental understanding of thermal conductivity.
- Organizing committee, 2013 APS Division of Fluid Dynamics Meeting.
- Outstanding Reviewer, 2015.
- *Physical Review B* ad hoc Editorial Board member: 2021, 2024.

MRS

- Member (2007-)
- Symposium organizer, 2011 MRS Spring Meeting. Co-organizers: Ming Su (U. Central Florida), Shawn Putnam (Air Force), Junichiro Shiomi (U. Tokyo).
- *MRS Bulletin* Guest Editor (with Davide Mattia), April 2017 issue on "Materials enabling nanofluidic flow enhancement."

Other Conference and Workshop Organization

- Co-organizer (with D. Leitner), Telluride Science Research Center June 2010 and June 2013 workshops "Thermal transport at the nanoscale," Telluride, CO.
- Organizer, May 2013 Harrington Symposium, "Next-generation materials for energy generation, storage, and transport," Austin, TX.
- Co-organizer (with D. Donadio), CECAM workshop "Advanced thermoelectrics at nanoscale: from materials to devices." Lugano, Switzerland, June 2011.
- Symposium organizer, "Characterization and modeling of ceramic-ceramic and metal-ceramic interfaces," Materials Science & Technology Conference, 2009. Co-organizers: Judith Yang (U. Pittsburgh), Susan Sinnott (U. Florida).
- Organizer of "Simulators' Meeting," Carnegie Mellon University, 2007-2011 & 2013-2018.

Other

- Reviewer for *ACS Nano, Annual Review of Heat Transfer, Applied Physics Letters, Communications in Nonlinear Science and Numerical Simulation, European Physics Letters, International Journal for Computational Methods in Engineering Science and Mechanics, International Journal of Heat and Fluid Flow, International Journal of Heat and Mass Transfer, Journal of Applied Physics, Journal of Chemical Physics, Journal of Heat Transfer, Journal of Physical Chemistry, Journal of Physical Chemistry Letters, Journal of Physics: Condensed Matter, Langmuir, Microfluidics and Nanofluidics, Nano Letters, Nanoscale, Nanoscale and Microscale Thermophysical Engineering, Nature, Nature Materials, Nature Nanotechnology, Nature Communications, New Journal of Physics, Physics of Fluids, Physical Review Applied, Physical Review B, Physical Review E, Physical Review Letters, Proceedings of the Royal Society A, Reviews of Modern Physics, Scientific Reports*, Department of Energy Office of Basic Energy Sciences, National Science Foundation, Army Research Lab, Office of Naval Research, Petroleum Research Fund.
- Panelist, graduate student workshop on obtaining an academic position, University of Michigan, November 2005, May 2015.

- Speaker for SWE High School Outreach, CMU, 2005-2009.
- YWCA TechGyrls coach, Fall 2008, Spring 2010, Spring 2011, Spring 2012.
- Osher Lifelong Learning Institute at CMU. Five-session short course in 2009. One lecture in 2016.
- Mattress Factory camp "Cartoons and Creations." Volunteer, Summer 2016